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Funding

Kinetic Modelling of the Pyrolysis and Oxidation of Furans

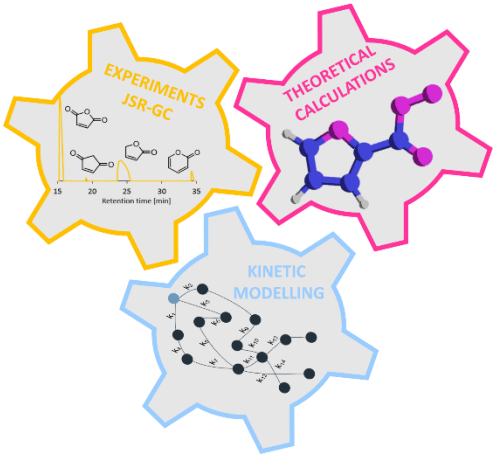
Aim

The aim of this master thesis is to develop a fundamental kinetic model for the pyrolysis and oxidation of furans. The study involves a combination of theoretical calculations, kinetic modelling and comparison to experimental work.

Justification

Furans are an important class of compounds present in bio-oil produced by biomass fast pyrolysis. In particular, the pyrolysis of the carbohydrate pulp in lignocellulose biomass forms a broad range of furans with oxygenated substituents. Many studies focus on the subsequent catalytic upgrading of the furans in bio-oil for the production of fuels and chemicals, but only few have studied the thermal decomposition of these furans. The decomposition chemistry depends on the presence of functional groups on the furan ring structure. For furan and furans with alkyl substituents, such as 2-methyl furan and 2,5-dimethyl furan the thermal decomposition has been studied thoroughly. Studies on furans with oxygenated substituents, on the other hand, are scarce. Furthermore, it was found experimentally that furfural oxidation results in the production of lactones, which are considered high-value chemicals. A kinetic modeling study on the oxidation of furfural can provide insights in the chemical mechanism required to optimize experimental conditions for the production of these high-value chemicals.

A kinetic model for the pyrolysis and oxidation of furans can be constructed automatically with the use of Genesys. It was found before that the thermal decomposition chemistry of furans is unique. New types of radical chemistry and reaction pathways were discovered through quantum chemical calculations, and those new reaction families have to be implemented in Genesys. On-the-fly fast estimation techniques for thermodynamic properties and kinetic parameters, such as group additivity, have to be adjusted to account for these new reaction pathways. For this reason, some thermodynamic and kinetic parameters will be determined with quantum mechanical techniques automatically with Genesys. Literature based or in-house developed experimental data will be used to extensively validate the developed kinetic model.



Program

- Literature survey regarding experimental and modelling studies for upgrading of furans.
- Collection and curation of experimental measurements and processing of available quantum chemical calculations.
- New experimental measurements for the pyrolysis of furans
- Automatic determination of new thermodynamic properties and reaction rate coefficients with *ab initio* techniques implemented in Genesys.
- Generation of a kinetic model for the model compounds automatically with Genesys.
- Reactor simulations to compare the results of the kinetic model to experimental data.

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